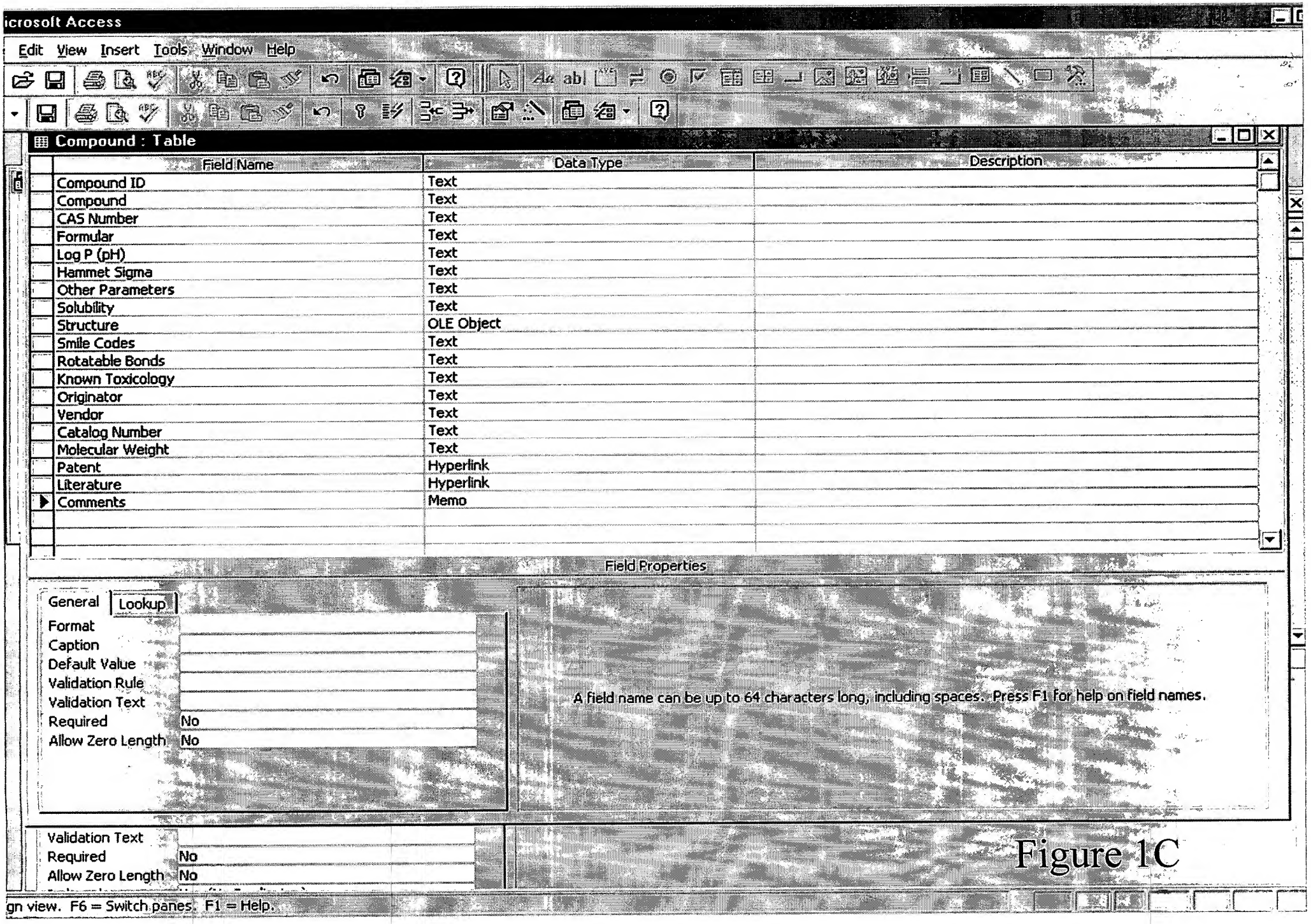

icrosoft Access
Edit View Insert Tools Window Help
Compound : Table
Field Name
Data Type
Description
Compound ID
Text
Compound
Text
CAS Number
Text
Formular
Text
Log P (pH)
Text
Hammet Sigma
Text
Other Parameters
Text
Solubility
Text
Structure
OLE Object
Smile Codes
Text
Rotatable Bonds
Text
Known Toxicology
Text
Originator
Text
Vendor
Text
Catalog Number
Text
Molecular Weight
Text
Patent
Hyperlink
Literature
Hyperlink
Comments
Memo
Field Properties
General
Lookup
Format
Caption
Default Value
Validation Rule
Validation Text
Required
No
Allow Zero Length
No
A field name can be up to 64 characters long, including spaces. Press F1 for help on field names.
Validation Text
Required
No
Allow Zero Length
No
gn view. F6 = Switch panes. F1 = Help.

Figure 1C

Three-component Database For Drug Discovery/Development

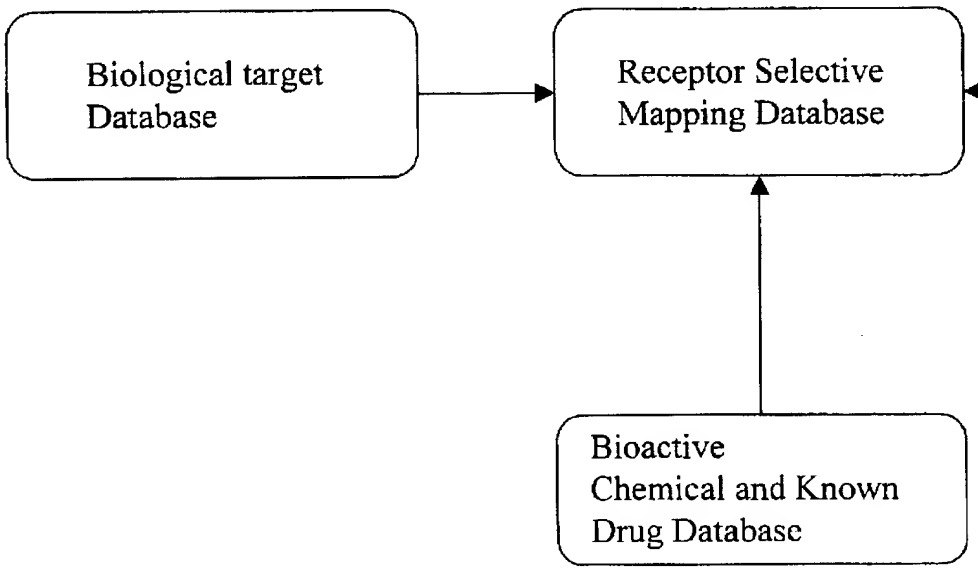


Chart 2

Compositional Matter - the RSM database contains three key components as indicated. All three contribute information into the RSM database. The biological target database includes all potential current and future drug targets, the biological database is comprised of the information about all physiological information of disease/healthy state, drug efficacy, side effects and toxicology. The bioactive chemical and known drug database contains chemicals that are know to be active against certain biological targets; useful in treating diseases.The chemical database also includes natural products in the form of biomass, extracts, or compounds that are not entirely from chemical synthetic origin.

FIG. 1D

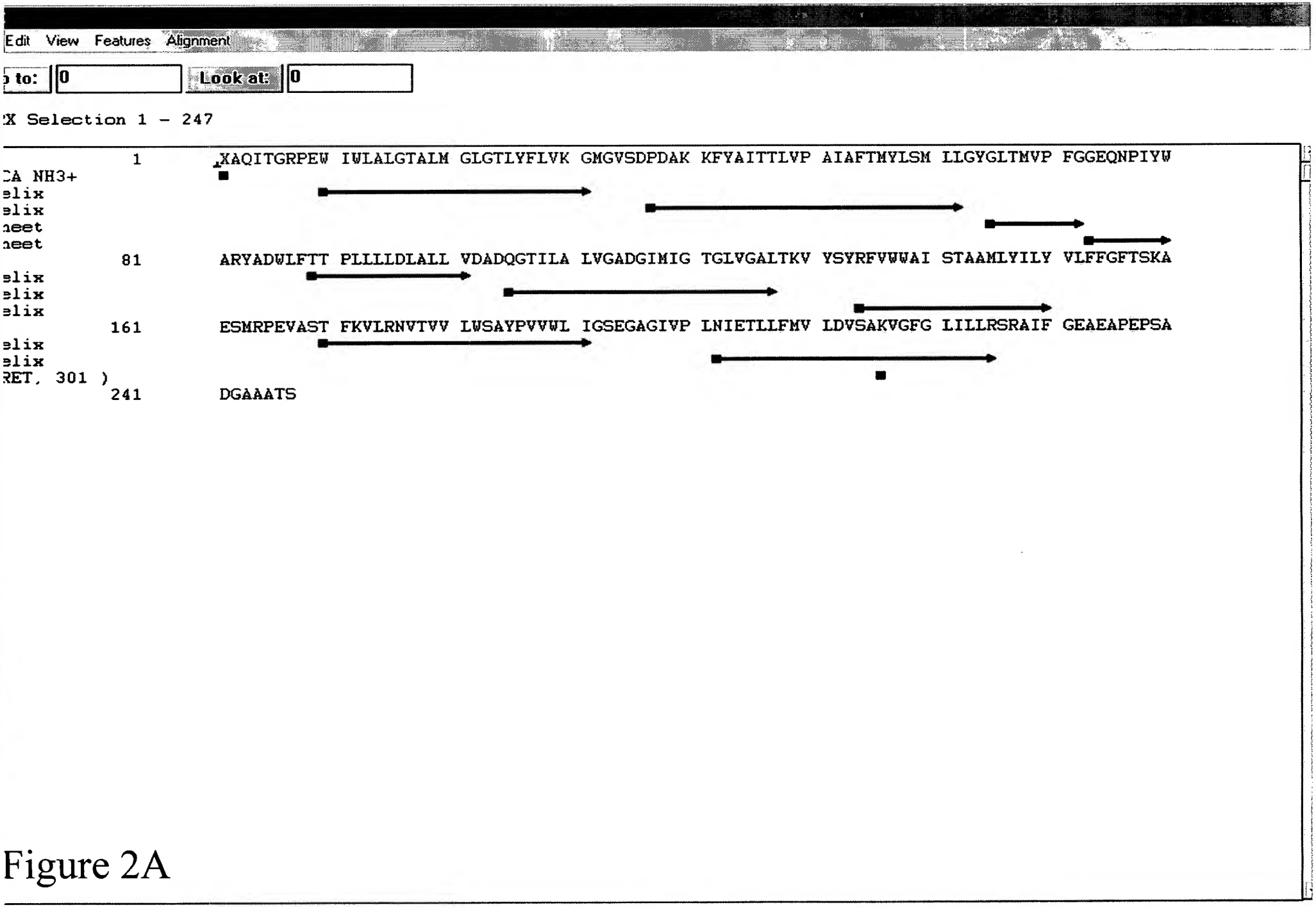

Edit View Features Alignment
to: 0
Look at: 0
X Selection 1 - 247
1 XAQITGRPEW IWLALGTALM GLGTLYFLVK GMGVSDPDAK KFYAITTLVP AIAFTMYLSM LLGYGLTMVP FGGEQNPIYW
CA NH3+
elix
elix
neet
neet
81 ARYADWLFTT PLLLLDLALL VDADQGTILA LVGADGIMIG TGLVGALTKV YSYRFVWWAI STAAMLYILY VLFFGFTSKA
elix
elix
elix
161 ESMRPEVAST FKVLRNVTVV LWSAYPVVWL IGSEGAGIVP LNIETLLFMV LDVSAKVGFG LILLRSRAIF GEAEAPEPSA
elix
elix
RET, 301)
241 DGAAATS

Figure 2A

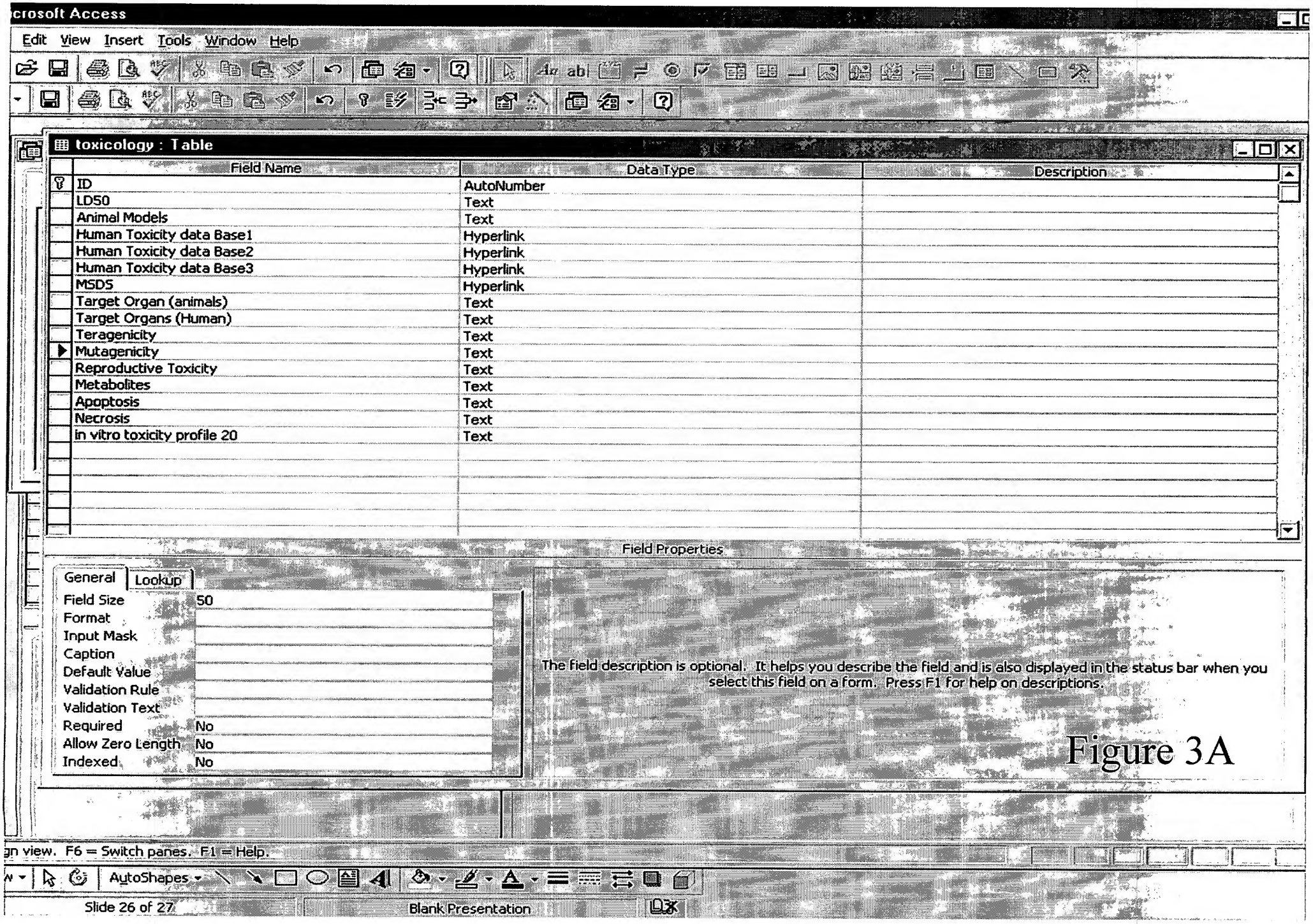
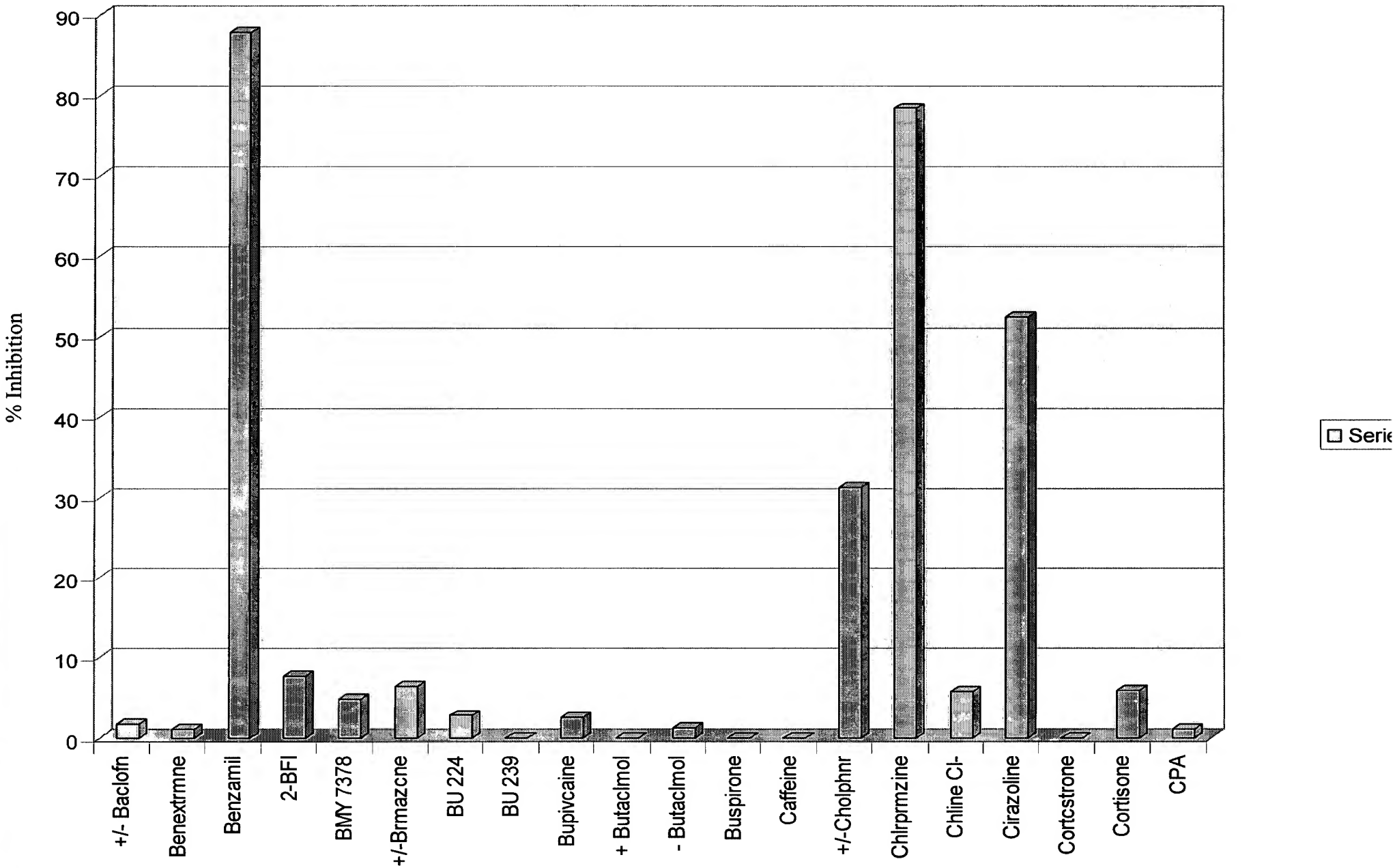

crosoft Access
Edit View Insert Tools Window Help
toxicology : Table
Field Name
Data Type
Description
ID
AutoNumber
LD50
Text
Animal Models
Text
Human Toxicity data Base1
Hyperlink
Human Toxicity data Base2
Hyperlink
Human Toxicity data Base3
Hyperlink
MSDS
Hyperlink
Target Organ (animals)
Text
Target Organs (Human)
Text
Teragenicity
Text
Mutagenicity
Text
Reproductive Toxicity
Text
Metabolites
Text
Apoptosis
Text
Necrosis
Text
in vitro toxicity profile 20
Text
Field Properties
General
Lookup
Field Size
50
Format
Input Mask
Caption
Default Value
Validation Rule
Validation Text
Required
No
Allow Zero Length
No
Indexed
No
The field description is optional. It helps you describe the field and is also displayed in the status bar when you select this field on a form. Press F1 for help on descriptions.
gn view. F6 = Switch panes. F1 = Help.
AutoShapes
Slide 26 of 27
Blank Presentation

Figure 3A

Figure 7A


Chemical profile - 5HT3
% Inhibition
90
80
70
60
50
40
30
20
10
0
+/- Baclofn
Benextrmne
Benzamil
2-BFI
BMY 7378
+/-Brmazcne
BU 224
BU 239
Bupivcaine
+ Butaclmol
- Butaclmol
Buspirone
Caffeine
+/-Cholphnr
Chlrprmzine
Chline Cl-
Cirazoline
Cortcstrone
Cortisone
CPA
Serie

Chemical Profile

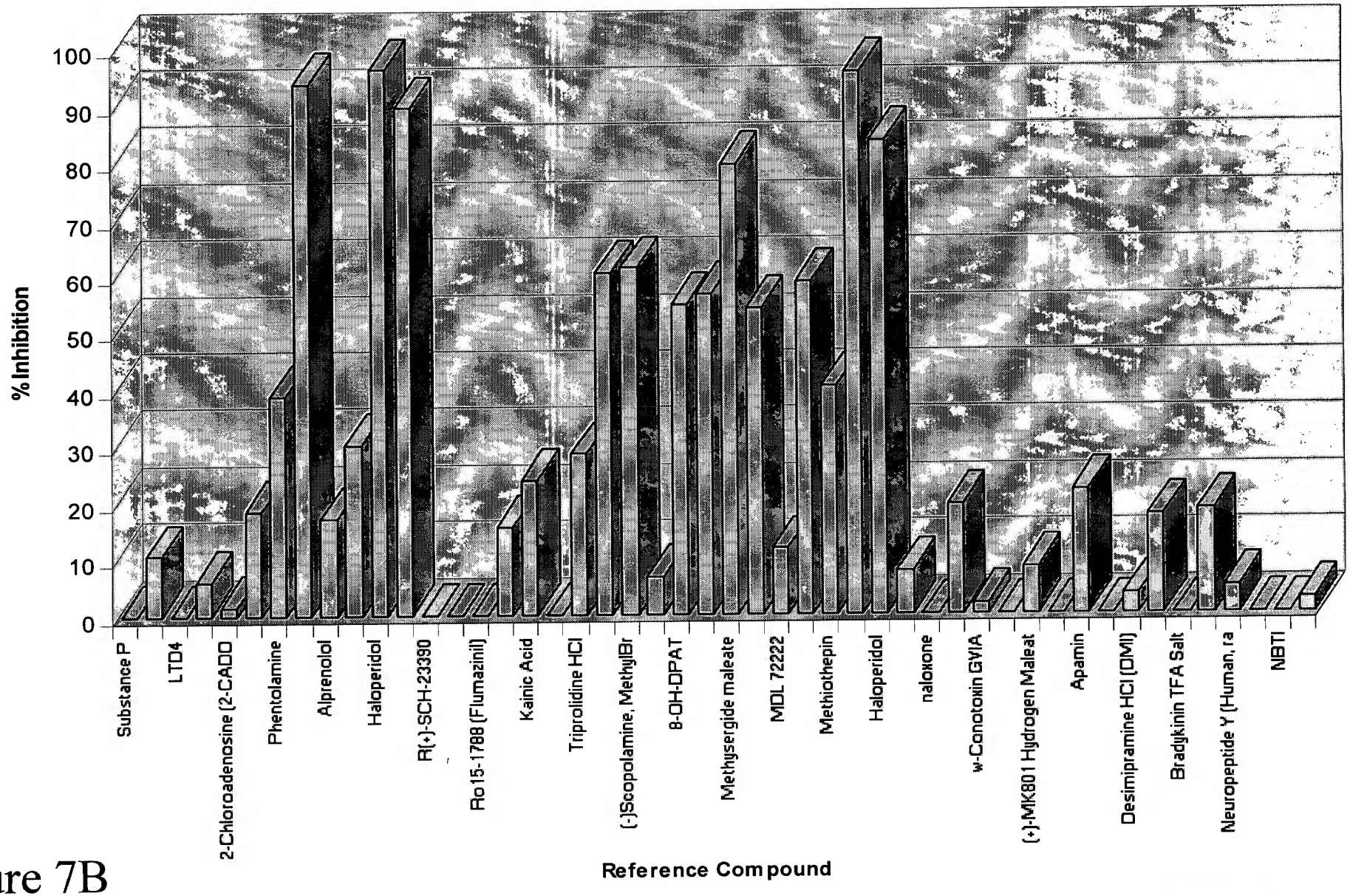


Figure 7B

Chemical Profiles

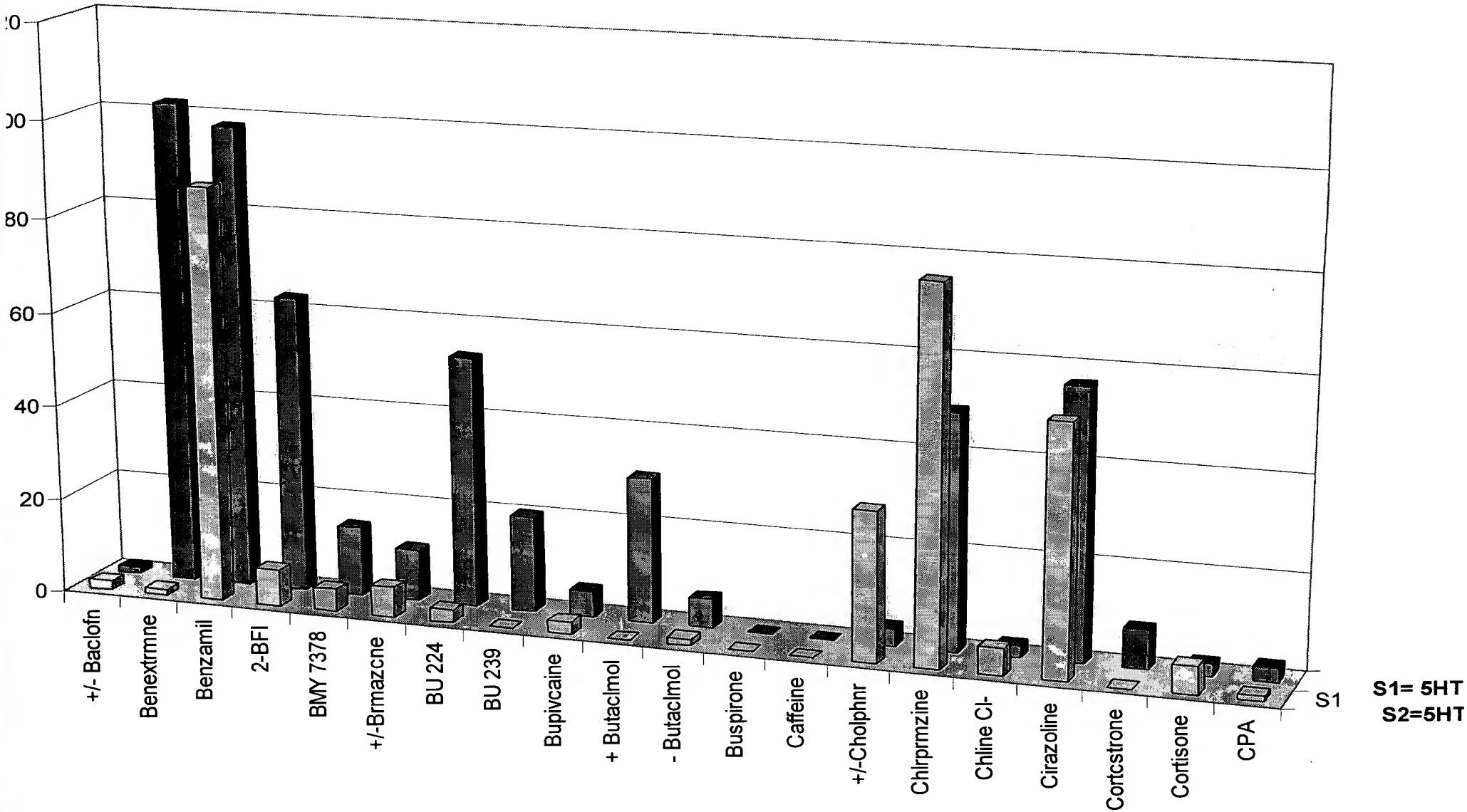


Figure 7C

Reference Compounds

Figure 8A

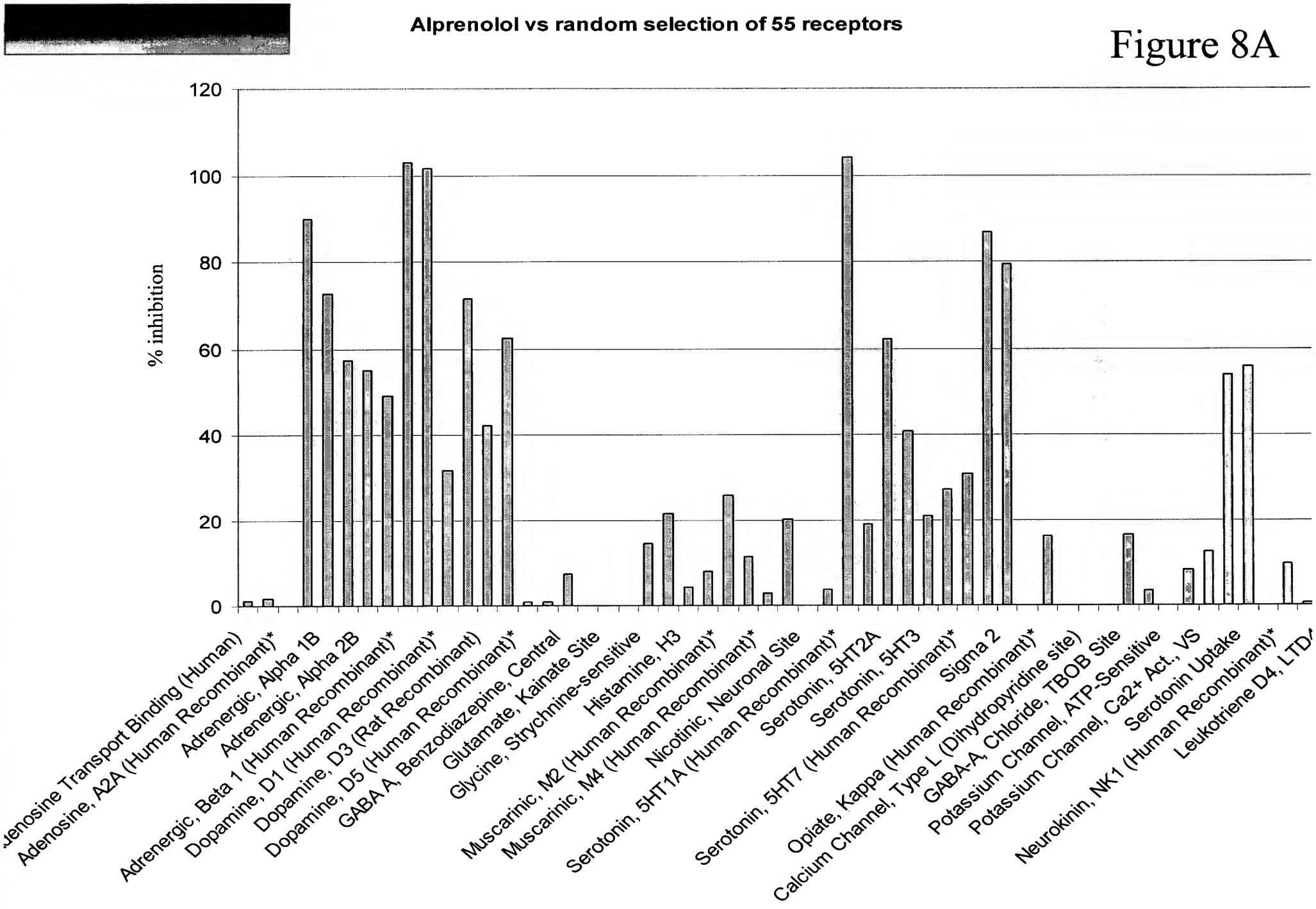
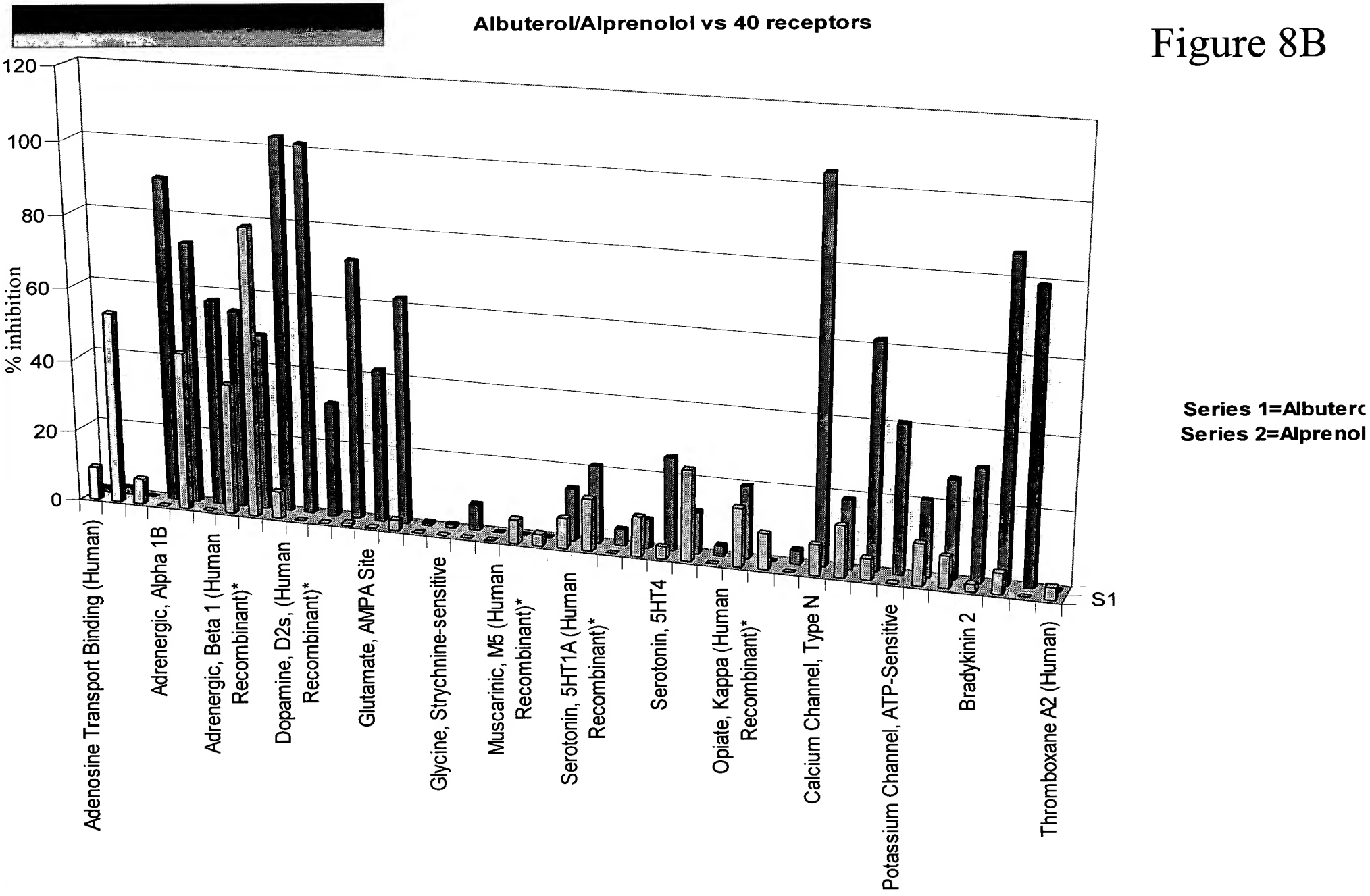

Alprenolol vs random selection of 55 receptors
% inhibition
120
100
80
60
40
20
0
Adenosine Transport Binding (Human)
Adenosine, A2A (Human Recombinant)*
Adrenergic, Alpha 1B
Adrenergic, Alpha 2B
Adrenergic, Beta 1 (Human Recombinant)*
Dopamine, D1 (Human Recombinant)*
Dopamine, D3 (Rat Recombinant)
Dopamine, D5 (Human Recombinant)*
GABA A, Benzodiazepine, Central
Glutamate, Kainate Site
Glycine, Strychnine-sensitive
Histamine, H3
Muscarinic, M2 (Human Recombinant)*
Muscarinic, M4 (Human Recombinant)*
Nicotinic, Neuronal Site
Serotonin, 5HT1A (Human Recombinant)*
Serotonin, 5HT2A
Serotonin, 5HT3
Serotonin, 5HT7 (Human Recombinant)*
Sigma 2
Opiate, Kappa (Human Recombinant)*
Calcium Channel, Type L (Dihydropyridine site)
GABA-A, Chloride, TBOB Site
Potassium Channel, ATP-Sensitive
Potassium Channel, Ca2+ Act., VS
Serotonin Uptake
Neurokinin, NK1 (Human Recombinant)*
Leukotriene D4, LTD

Figure 8B


Albuterol/Alprenolol vs 40 receptors
120
100
80
60
40
20
0
% inhibition
Adenosine Transport Binding (Human)
Adrenergic, Alpha 1B
Adrenergic, Beta 1 (Human Recombinant)*
Dopamine, D2s, (Human Recombinant)*
Glutamate, AMPA Site
Glycine, Strychnine-sensitive
Muscarinic, M5 (Human Recombinant)*
Serotonin, 5HT1A (Human Recombinant)*
Serotonin, 5HT4
Opiate, Kappa (Human Recombinant)*
Calcium Channel, Type N
Potassium Channel, ATP-Sensitive
Bradykinin 2
Thromboxane A2 (Human)
S1
Series 1=Albuterc
Series 2=Alprenol